

Stationary Probability Vectors of Higher-order Markov Chains

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Abstract

In this note, we consider the higher-order Markov Chain, and characterize the second order Markov chains admitting every probability distribution vector as a stationary vector. The result is used to construct Markov chains of higher-order with the same property. We also study conditions under which the set of stationary vectors of the Markov chain has a certain affine dimension.

Key words. Transition probability tensor, higher-order Markov chains.

1 Introduction

A discrete-time Markov chain is a stochastic process with a sequence of random variables

$$\{X_t, t = 0, 1, 2, \dots\},$$

which takes on values in a discrete finite state space

$$\langle n \rangle = \{1, \dots, n\}$$

for a positive integer n , such that with time independent probability

$$\begin{aligned} p_{ij} &= \Pr(X_{t+1} = i | X_t = j, X_{t-1} = i_{t-1}, X_{t-2} = i_{t-2}, \dots, X_1 = i_1, X_0 = i_0) \\ &= \Pr(X_{t+1} = i | X_t = j) \end{aligned}$$

holds for all $i, j, i_0, \dots, i_{t-1}$. The nonnegative matrix $P = (p_{ij})_{1 \leq i, j \leq n}$ is the transition matrix of the Markov process is column stochastic, i.e., $\sum_{i=1}^n p_{ij} = 1$ for $j = 1, \dots, n$. Denote by

$$\Omega_n = \left\{ \mathbf{x} = (x_1, \dots, x_n)^t : x_1, \dots, x_n \geq 0, \sum_{i=1}^n x_i = 1 \right\} \quad (1)$$

the simplex of probability vectors in \mathbf{R}^n . A nonnegative vector $\mathbf{x} \in \Omega_n$ is a stationary probability vector (also known as the distribution) of a finite Markov Chain if $P\mathbf{x} = \mathbf{x}$. By the Perron-Frobenius Theory (e.g., see [3, 8]) every discrete-time Markov Chain has a stationary probability vector, and the vector is unique if the transition matrix is primitive, i.e., there is a positive integer r such that all entries of P^r are positive. The uniqueness condition is useful when one uses numerical schemes

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to determine the stationary vectors. With the uniqueness condition, any convergent scheme would lead to the unique stationary vector; e.g., see [4].

More generally, one may consider an m -th order Markov chain such that

$$\begin{aligned} p_{i,i_1,\dots,i_m} &= \Pr(X_{t+1} = i | X_t = i_1, X_{t-1} = i_2, \dots, X_1 = i_t, X_0 = i_{t+1}) \\ &= \Pr(X_{t+1} = i | X_t = i_1, \dots, X_{t-m+1} = i_m), \end{aligned}$$

where $i, i_1, \dots, i_m \in \langle n \rangle$; see [1, 2]. In other words, the current state of the process depends on m past states. Observe that

$$\sum_{i=1}^n p_{i,i_1,\dots,i_m} = 1, \quad 1 \leq i_1, \dots, i_m \leq n.$$

When $m=1$, it is just the standard Markov Chain. There are many situations that one would use the Markov Chain models. We refer readers to the papers [1, 2, 5, 6, 7] and the references therein. Note that $P = (p_{i,i_1,\dots,i_m})$ is an $(m+1)$ -fold tensor of \mathbf{R}^n governing the transition of states in the m -th order Markov chain according to the following rule

$$x_i(t+1) = \sum_{1 \leq i_1, \dots, i_m \leq n} p_{i,i_1,\dots,i_m} x_{i_1}(t) \cdots x_{i_m}(t), \quad i = 1, \dots, n.$$

We will call P the transition probability tensor of the Markov chain. A nonnegative vector $\mathbf{x} = (x_1, \dots, x_n)^t \in \mathbf{R}^n$ with entries summing up to 1 is a stationary (probability distribution) vector if

$$x_i = \sum_{1 \leq i_1, \dots, i_m \leq n} p_{i,i_1,\dots,i_m} x_{i_1} \cdots x_{i_m}, \quad i = 1, \dots, n. \quad (2)$$

In [5] the authors used a fixed point theorem to show that a stationary vector for a higher-order Markov chain always exists; the stationary vector will have positive entries if the transition tensor $P = (p_{i,i_1,\dots,i_m})$ is irreducible, i.e., there is no non-empty proper index subset $I \subset \{1, 2, \dots, n\}$ such that $p_{i,i_1,\dots,i_m} = 0$ for all $i \in I$, and $i_1, \dots, i_m \notin I$. Moreover, they derived some sufficient conditions for the stationary vector to be unique, and proposed some iterative methods to find the stationary vector. As mentioned before, the uniqueness of the stationary vector is important in using iterative methods to find stationary vectors.

In this note, we consider an extreme situation of the problem, namely, every probability vector in the simplex Ω_n is a stationary vector of a higher-order Markov chain. In the standard (first-order) Markov chain, this can happen if and only if P is the identity matrix. We show that such a phenomenon may occur for a large family of higher-ordered Markov chains. In particular, we characterize those second order Markov chains with this property. The result is used to study higher-order Markov chains with the same property.

In our discussion, we always let

$$\mathcal{E} = \{e_1, \dots, e_n\}$$

denote the standard basis for \mathbf{R}^n . Then Ω_n is the convex hull of the set \mathcal{E} . For any $k \in \{1, \dots, n\}$, a subset of Ω_n obtained by taking the convex hull of k vectors from the set \mathcal{E} is a face of the simplex Ω_n of affine dimension $k-1$. We also consider higher-order Markov chains with a $(k-1)$ -dimension face of Ω_n as the set of stationary vectors. Other geometrical features and problems concerning the set of stationary vectors of higher-order Markov chains will also be mentioned.

2 Second Order Markov Chains

In the following, we characterize those second order Markov chains so that every vector in Ω_n is a stationary vector. Note that for a second order Markov chains the conditions for the stationary vector $\mathbf{x} = (x_1, \dots, x_n)^t$ in (2) can be rewritten as

$$\mathbf{x} = (x_1 P_1 + \dots x_n P_n) \mathbf{x}, \quad (3)$$

where for $i = 1, \dots, n$,

$$P_i = (p_{ris})_{1 \leq r, s \leq n} \quad (4)$$

is a column stochastic matrix, i.e., a nonnegative matrix so that the sum of entries of each column is 1. We have the following theorem.

Theorem 2.1 *Suppose $P = (p_{i,i_1,i_2})$ is the transition tensor of a second order Markov chain. Then every vector in the set Ω_n is a stationary vector if and only if there are nonnegative vectors $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbf{R}^n$ with entries in $[0, 1]$ such that for $i = 1, \dots, n$, $\mathbf{v}_i = (v_{i1}, \dots, v_{in})^t$ with $v_{ii} = 0$, and*

$$P_i = I_n - \text{diag}(v_{i1}, \dots, v_{in}) + e_i \mathbf{v}_i^t = \begin{pmatrix} 1 - v_{i1} & & & & & & \\ & \ddots & & & & & \\ & & 1 - v_{i,i-1} & & & & \\ v_{i1} & \cdots & v_{i,i-1} & 1 & v_{i,i+1} & \cdots & v_{in} \\ & & & 1 - v_{i,i+1} & & & \\ & & & & \ddots & & \\ & & & & & & 1 - v_{in} \end{pmatrix}.$$

To prove Theorem 2.1, we need the following detailed analysis for the second order Markov chain when $n = 2$.

Proposition 2.2 *Let $a_1, a_2, b_1, b_2 \in [0, 1]$. Consider the following equation with unknown $x \in [0, 1]$:*

$$\left[x \begin{pmatrix} a_1 & b_1 \\ 1 - a_1 & 1 - b_1 \end{pmatrix} + (1 - x) \begin{pmatrix} a_2 & b_2 \\ 1 - a_2 & 1 - b_2 \end{pmatrix} \right] \begin{pmatrix} x \\ 1 - x \end{pmatrix} = \begin{pmatrix} x \\ 1 - x \end{pmatrix}.$$

Then one of the following holds for the above equation.

- (1) *If $a_1 = 1, a_2 + b_1 = 1, b_2 = 0$, then every $x \in [0, 1]$ is a solution.*
- (2) *If $a_2 + b_1 < 1 = a_1$, then there are two solutions in $[0, 1]$, namely, $x = 1$ and $x = \frac{b_2}{b_2 + 1 - a_2 - b_1}$.*
- (3) *If $a_2 + b_1 - a_1 > a_2 + b_1 - 1 \geq 0 = b_2$, then there are two solutions in $[0, 1]$, namely, $x = 0$ and $x = \frac{a_2 + b_1 - 1}{a_2 + b_1 - a_1}$.*
- (4) *Otherwise, there is a unique solution in $[0, 1]$ determined as follows.*
If $a_1 - a_2 - b_1 + b_2 = 0$, then $x = \frac{b_2}{2b_2 + 1 - a_2 - b_1}$.

If $a_1 - a_2 - b_1 + b_2 \neq 0$, then

$$x = \frac{2b_2 + 1 - a_2 - b_1 - \sqrt{\Delta}}{2(a_1 - a_2 - b_1 + b_2)}$$

with $\Delta = (2b_2 + 1 - a_2 - b_1)^2 - 4b_2(a_1 - a_2 - b_1 + b_2) = (1 - a_2 - b_1)^2 + 4b_2(1 - a_1) \geq 0$.

Proof. Let

$$f(x) = (a_1 - a_2 - b_1 + b_2)x^2 + (a_2 + b_1 - 2b_2)x + b_2$$

be the first entry of the vector

$$\left[x \begin{pmatrix} a_1 & b_1 \\ 1 - a_1 & 1 - b_1 \end{pmatrix} + (1 - x) \begin{pmatrix} a_2 & b_2 \\ 1 - a_2 & 1 - b_2 \end{pmatrix} \right] \begin{pmatrix} x \\ 1 - x \end{pmatrix}.$$

We need only solve $f(x) = x$ with $x \in [0, 1]$. Then the equation corresponding to the second entry will also satisfy. Set

$$g(x) = f(x) - x = (a_1 - a_2 - b_1 + b_2)x^2 + (a_2 + b_1 - 2b_2 - 1)x + b_2 = 0.$$

Then $g(0) = b_2 \geq 0$ and $g(1) = a_1 - 1 \leq 0$. By the Intermediate Value Theorem, there is at least one $x_0 \in [0, 1]$ such that $g(x_0) = 0$. Let

$$\Delta = (2b_2 + 1 - a_2 - b_1)^2 - 4b_2(a_1 - a_2 - b_1 + b_2) = (1 - a_2 - b_1)^2 + 4b_2(1 - a_1) \geq 0.$$

Suppose $a_1 - a_2 - b_1 + b_2 = 0$. The quadratic equation reduces to $(a_2 + b_1 - 2b_2 - 1)x + b_2 = 0$. If $a_2 + b_1 - 2b_2 - 1 = 0$, then one can readily check that condition (1) holds. If $a_2 + b_1 - 2b_2 - 1 \neq 0$, then the first case of condition (4) holds.

Suppose $a_1 - a_2 - b_1 + b_2 \neq 0$. If $g(0) > 0$ and $g(1) < 0$, then the quadratic function $g(x)$ can only have one solution in $[0, 1]$. If $a_1 - a_2 - b_1 + b_2 > 0$, then $g(x) \rightarrow \infty$ as $x \rightarrow \infty$. Since $g(1) < 0$, the larger root of $g(x) = 0$ equals $\frac{2b_2 + 1 - a_2 - b_1 + \sqrt{\Delta}}{2(a_1 - a_2 - b_1 + b_2)}$ will be larger than 1. Hence, the second case of condition (4) holds. If $a_1 - a_2 - b_1 + b_2 < 0$, then $g(x) \rightarrow -\infty$ as $x \rightarrow -\infty$. Since $g(0) > 0$, the smaller root of $g(x) = 0$ equals $\frac{2b_2 + 1 - a_2 - b_1 + \sqrt{\Delta}}{2(a_1 - a_2 - b_1 + b_2)}$ will be smaller than 0. Hence, the second case of condition (4) holds.

Suppose $0 = g(1) = a_1 - 1$. Then $g(x)$ will have another solution in $[0, 1]$ if and only if $a_1 - a_2 - b_1 + b_2 = 1 - a_2 - b_1 + b_2 \geq 0$. This happens if and only if condition (2) holds.

Suppose $0 = g(0) = b_2$ and $0 \neq g(1)$. Then $g(x)$ will have another solution in $[0, 1]$ if and only if $a_1 - a_2 - b_1 + b_2 = a_1 - a_2 - b_1 < 0$ and the maximum of $g(x)$ is attained at a positive number x . This happens if and only if condition (3) holds. \square

Proof of Theorem 2.1. The sufficiency can be readily checked. We focus on the necessity. Note that Proposition 2.2 covers the case when $n = 2$. We will use an inductive argument. It is illustrative to see the case when $n = 3$. Consider the system

$$\left[x_1 \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} + x_2 \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix} + x_3 \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix} \right] \mathbf{x} = \mathbf{x}.$$

If we set the third entry of the stationary vector \mathbf{x} to be 0, then we can have infinitely many solutions of the form $\mathbf{x} = \begin{pmatrix} x \\ 1-x \\ 0 \end{pmatrix}$ with $x \in [0, 1]$. By the 2-by-2 case, this happens if and only if the sub-matrices $\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ and $\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$ are of the form $\begin{pmatrix} 1 & a_{12} \\ 0 & 1-a_{12} \end{pmatrix}, \begin{pmatrix} 1-a_{12} & 0 \\ a_{12} & 1 \end{pmatrix}$. Similarly, setting the second entry of \mathbf{x} to be 0, we see that the submatrices $\begin{pmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{pmatrix}$ and $\begin{pmatrix} c_{11} & c_{13} \\ c_{31} & c_{33} \end{pmatrix}$ are of the form $\begin{pmatrix} 1 & a_{13} \\ 0 & 1-a_{13} \end{pmatrix}, \begin{pmatrix} 1-a_{13} & 0 \\ a_{13} & 1 \end{pmatrix}$. Finally, setting the first entry of \mathbf{x} to be 0, we see that the sub-matrices $\begin{pmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{pmatrix}$ and $\begin{pmatrix} c_{22} & c_{23} \\ c_{32} & c_{33} \end{pmatrix}$ are of the form $\begin{pmatrix} 1 & a_{23} \\ 0 & 1-a_{23} \end{pmatrix}, \begin{pmatrix} 1-a_{23} & 0 \\ a_{23} & 1 \end{pmatrix}$. Thus, the three matrices in the equation are of the form

$$\begin{pmatrix} 1 & a_{12} & a_{13} \\ 0 & 1-a_{12} & 0 \\ 0 & 0 & 1-a_{13} \end{pmatrix}, \begin{pmatrix} 1-a_{12} & 0 & 0 \\ a_{12} & 1 & a_{23} \\ 0 & 0 & 1-a_{23} \end{pmatrix}, \begin{pmatrix} 1-a_{13} & 0 & 0 \\ 0 & 1-a_{23} & 0 \\ a_{13} & a_{23} & 1 \end{pmatrix}.$$

More generally, suppose the result holds for the $(n-1)$ -dimension case. Consider the n -dimension case, and the equation

$$(x_1 P_1 + \cdots + x_n P_n) \mathbf{x} = \mathbf{x} \quad \text{with } \mathbf{x} \in \Omega_n.$$

Let $j \in \{1, \dots, n\}$. Setting the j -th entry of $\mathbf{x} = (x_1, \dots, x_n)^t$ to be zero, we see that for $i \neq j$, the $(n-1)$ sub-matrix of P_i obtained by deleting its j th row and j th column has the form

$$I_{n-1} - \text{diag}(a_{i,1}, \dots, a_{i,j-1}, a_{i,j+1}, \dots, a_{i,n}) + \hat{e}_i(a_{i,1}, \dots, a_{i,j-1}, a_{i,j+1}, \dots, a_{i,n}),$$

where \hat{e}_i is obtained from e_i by removing the j th entry for $i = 1, \dots, n$. Combining the information for different $j = 1, \dots, n$, and $i = 1, \dots, j-1, j+1, \dots, n$, we see that the matrices P_1, \dots, P_n have the asserted form. \square

Theorem 2.1 shows that it is possible for a second order Markov chain to have many stationary vectors. In [5], the authors obtained some sufficient conditions for a higher-order Markov chain to have a unique stationary vector. Here we construct a family of examples of second-order Markov chains such that one of the following holds.

- (a) There are exactly k stationary vectors for a given $k \in \{1, \dots, n+1\}$.
- (b) The set of stationary vectors is a k dimensional face of Ω_n for $k = 1, \dots, n-2$.
- (c) The set of stationary vectors is a disconnected set equal to the union of a k dimensional face of Ω_n and $\{(\sum_{j=1}^n e_j)/n\}$, for $k = 1, \dots, n-2$.

Theorem 2.3 *Suppose $n > 2$ and a second order Markov chain with transition tensor $P = (p_{i,i_1,i_2})$. Let $P_i = (p_{ris})_{1 \leq r,s \leq n}$ for $i = 1, \dots, n$. Let $k \in \{1, \dots, n\}$ and $f_k = (e_1 + \cdots + e_k)/k$. If every column of P_i equals f_k , then f_k is the only stationary vector of the Markov chain.*

- (1) If $k = 2$, replace the first column of P_1 by e_1 and all the columns of P_2 by e_2 . Then the resulting Markov chain has 2 stationary vectors, namely, e_1 and e_2 .
- (2) If $2 < k \leq n$, replace the i th column of P_i by e_i and all other columns by e_k for $i = 1, \dots, k$. Then the resulting Markov chain has k stationary vectors, namely, e_1, \dots, e_k .
- (3) Suppose $k = n$. If we replace the i th column of P_i by e_i and all $i = 1, \dots, n$, then the resulting Markov chain has $n + 1$ stationary vectors, namely, e_1, \dots, e_n and f_n .
- (4) If $k \in \{2, \dots, n - 1\}$ and we replace the first k columns of P_i by e_i for $i = 1, \dots, k$, then the set of stationary vectors for the Markov chain equals the convex hull of $\{e_1, \dots, e_k\}$.
- (5) Suppose $k \in \{2, \dots, n - 1\}$ and we reset the matrices P_1, \dots, P_n so that the first k columns of P_i equal

$$v_i = \begin{cases} e_i & \text{if } i = 1, \dots, k, \\ (e_{k+1} + \dots + e_n)/(n - k) & \text{if } i = k+1, \dots, n, \end{cases}$$

and all other columns equal to f_n . Then the set of stationary vectors for the Markov chain equals the union of the convex hull of $\{e_1, \dots, e_k\}$ the set $\{f_n\}$.

Proof. Suppose $k \in \{1, \dots, n\}$ and every column of P_i equals f_k . Then $\mathbf{x} = (x_1, \dots, x_n)^t \in \Omega_n$ satisfies

$$\mathbf{x} = (x_1 P_1 + \dots + x_n P_n) \mathbf{x} = (x_1 + \dots + x_k) f_k$$

if and only if $x_{k+1} = \dots = x_n = 0$ and $x_1 = \dots = x_k = 1/k$.

- (1) Suppose $k = 2$, and we replace P_1 and P_2 as suggested. Then $\mathbf{x} \in \Omega_n$ satisfies

$$\mathbf{x} = (x_1 P_1 + \dots + x_n P_n) \mathbf{x}$$

if and only if $x_3 = \dots = x_n = 0$ and

$$x_1 \begin{pmatrix} 1 & 1/2 \\ 0 & 1/2 \end{pmatrix} + x_2 \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

By Proposition 2.2, $x_1 = 1$ or $x_2 = 1$. So, the Markov chain has two stationary vectors e_1 and e_2 .

(2) Suppose $k > 2$, and the i th column of P_i is replaced by e_i and replace all other columns by e_k for $i = 1, \dots, k$. Direct checking shows that e_1, \dots, e_k and f_k are stationary vectors of the Markov chain. Conversely, suppose $\mathbf{x} = (x_1, \dots, x_n)^t \in \Omega_n$ satisfies

$$\mathbf{x} = (x_1 P_1 + \dots + x_n P_n) \mathbf{x}.$$

Then $x_{k+1} = \dots = x_n = 0$,

$$x_k = \sum_{j=1}^{k-1} x_j (1 - x_j) + x_k, \quad \text{and} \quad x_j = x_j^2 \quad \text{for } j = 1, \dots, k-1.$$

Thus, $x_j \in \{0, 1\}$ so that $\mathbf{x} = e_j$ if $x_j = 1$ for any $j = 1, \dots, k-1$. If $x_1 = \dots = x_{k-1} = 0$, then x_k is the only nonzero entry and $\mathbf{x} = e_k$.

(3) Suppose $k = n$ and we replace the i th column of P_i by e_i and all $i = 1, \dots, n$. Direct computation shows that e_1, \dots, e_n and f_n are stationary vectors. Conversely, suppose $\mathbf{x} = (x_1, \dots, x_n)^t \in \Omega_n$ satisfies

$$\mathbf{x} = (x_1 P_1 + \dots + x_n P_n) \mathbf{x}.$$

Then

$$x_i = \frac{1}{n} \left(\sum_{1 \leq i, j \leq n} x_i x_j - \sum_{j=1}^k x_j^2 \right) + x_i^2 = \frac{1}{n} \left(1 - \sum_{j=1}^k x_j^2 \right) + x_i^2.$$

Let $\ell = \frac{1}{n} \left(1 - \sum_{j=1}^k x_j^2 \right)$ and consider two cases.

Case 1. If $\ell = 0$, then $x_i \in \{0, 1\}$ for each $i = 1, \dots, n$. Thus, we have $\mathbf{x} \in \{e_1, \dots, e_n\}$.

Case 2. Suppose $\ell > 0$. Because $x_i^2 - x_i + \ell = 0$, we see that $x_i = (1 \pm \sqrt{1 - 4\ell})/2$. If at least one of the x_i 's equals $(1 + \sqrt{1 - 4\ell})/2$, then by the fact that $n > 2$,

$$1 = \sum_{j=1}^n x_j \geq \frac{(1 + \sqrt{1 - 4\ell})}{2} + (n-1) \frac{(1 - \sqrt{1 - 4\ell})}{2} = 1 + (n-2) \frac{(1 - \sqrt{1 - 4\ell})}{2} > 1,$$

which is a contradiction. Thus, $x_i = (1 - \sqrt{1 - 4\ell})/2$ for each $i = 1, \dots, n$, and hence $\mathbf{x} = f_n$.

(4) Clearly, every vector in the convex hull of $\{e_1, \dots, e_k\}$ is a stationary vector of the Markov chain. Conversely, suppose $\mathbf{x} = (x_1, \dots, x_n)^t \in \Omega_n$ is a stationary vector. Then

$$\mathbf{x} = (x_1 P_1 + \dots + x_n P_n) \mathbf{x}$$

implies that $x_{k+1} = \dots = x_n = 0$, and x_1, \dots, x_k can be any nonnegative numbers summing up to one.

(5) One readily checks that f_n and every vector in the convex hull of $\{e_1, \dots, e_k\}$ is a stationary vector of the Markov chain. Conversely, suppose $\mathbf{x} = (x_1, \dots, x_n)^t \in \Omega_n$ is a stationary vector. If $\beta = (\sum_{j=k+1}^n x_j)$, then

$$\begin{aligned} \mathbf{x} &= (x_1 P_1 + \dots + x_n P_n) \mathbf{x} \\ &= (1 - \beta)(x_1 e_1 + \dots + x_k e_k) + \beta f_n + (1 - \beta)\beta(e_{k+1} + \dots + e_n)/(n - k). \end{aligned}$$

Thus, $x_{k+1} = \dots = x_n$. If all of them are zero, then x_1, \dots, x_k can be any nonnegative numbers summing up to one. If $x_{k+1} = \dots = x_n = r > 0$, then $x_i = (1 - \beta)x_i + \beta/n$ so that $x_i = 1/n$ for $i = 1, \dots, k$. It follows that $x_{k+1} = \dots = x_n = r = 1/n$ also. \square

Next, we obtain a result illustrating some additional geometrical feature of the set of stationary vectors of a second order Markov chain.

Proposition 2.4 *Consider the following equation for the stationary vectors of a second order Markov chain:*

$$(x_1 P_1 + \cdots + x_n P_n) \mathbf{x} = \mathbf{x}.$$

Suppose the Markov chain has two stationary vector of the form $xe_i + (1-x)e_j$ and $ye_i + (1-y)e_j$ for some $x, y \in (0, 1)$ and $1 \leq i < j \leq n$. Then every vector of the form $ze_i + (1-z)e_j$ with $z \in [0, 1]$ is a stationary vector of the Markov chain.

Proof. If $n = 2$, the result follows from Proposition 2.2. Suppose $n \geq 3$. The hypothesis of the proposition implies that the 2-by-2 submatrices of P_i and P_j lying in rows and columns indexed by i and j have the form $\begin{pmatrix} 1 & a \\ 0 & 1-a \end{pmatrix}$ and $\begin{pmatrix} 1-a & 0 \\ a & 1 \end{pmatrix}$. It follows that every vector of the form $ze_i + (1-z)e_j$ with $z \in [0, 1]$ is a stationary vector of the Markov chain. \square

Proposition 2.4 asserts that if the set of stationary vectors of a second order Markov chain contains two interior points of a 1-dimensional face of Ω_n , then every vector in the 1-dimensional face is a stationary vector.

We conjecture that if the set of stationary vectors of a second order Markov chain contains k interior points of a $(k-1)$ dimensional face of the simplex Ω_n , then every vector in the $(k-1)$ dimensional face is a stationary vector.

3 Higher-Order Markov Chains

In this section, we use the results in Section 2 to construct higher-order Markov chains so that

- (I) every vector in Ω_n is a stationary vector, and
- (II) the set of stationary vectors have different affine dimensions.

We will identify a transition probability tensor $P = (p_{i,i_1,\dots,i_m})$ as an $n \times n^m$ matrix with row index $i = 1, \dots, n$, and column indexes $i_1 \cdots i_m$ with $i_1, \dots, i_m \in \langle n \rangle = \{1, \dots, n\}$ arranged in lexicographic order. For example, for $n = 2$ and $m = 3$, the row indexes are 1, 2, and the column indexes are 111, 112, 121, 122, 211, 212, 221, 222. We will use the tensor (Kronecker) product notation for vectors in Ω_n . For example,

$$\mathbf{x}^{(3)} = \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x} = (x_1 x_1 x_1, x_1 x_1 x_2, x_1 x_2 x_1, x_1 x_2 x_2, x_2 x_1 x_1, x_2 x_1 x_2, x_2 x_2 x_1, x_2 x_2 x_2)^t.$$

The stationary vector condition can be represented as the following matrix equation:

$$P \mathbf{x}^{(m)} = \mathbf{x}.$$

We first consider Markov chains satisfying condition (I). We will illustrate the construction for the third order Markov chains for $n = 2$, and then describe the general construction.

First order Markov chains. Every vector in Ω_n is a stationary vector if and only if $P = I_2$.

Second order Markov chains. We can use the construction for the first order chain $P = I_2$ to produce the following.

$$[P|P]\mathbf{x} = \begin{pmatrix} p_{111} & p_{112} & p_{121} & p_{122} \\ p_{211} & p_{212} & p_{221} & p_{222} \end{pmatrix} \mathbf{x}^{(2)} = \mathbf{x} \quad \text{with } \mathbf{x} = (x_1x_1, x_1x_2, x_2x_1, x_2x_2)^t.$$

So, $Q = [P|P] = [I_2|I_2]$ satisfies $Q\mathbf{x}^{(2)} = \mathbf{x}$ for every $\mathbf{x} \in \Omega$. Observe that the second and third entries on $\mathbf{x}^{(2)}$ are the same, so one can permute the second the third columns of $[P, P]$ to get $\tilde{Q} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}$ such that $\tilde{Q}\mathbf{x}^{(2)} = \mathbf{x}$ for every $\mathbf{x} \in \Omega$. Evidently, for every $a \in [0, 1]$, $Q_a = aQ + (1-a)\tilde{Q}$ will satisfy $Q_a\mathbf{x}^{(2)} = \mathbf{x}$. In fact, we have shown that these are all possible transition tensors have the desired property.

Third order Markov chains. Suppose $Q = \begin{pmatrix} q_{111} & q_{112} & q_{121} & q_{122} \\ q_{211} & q_{212} & q_{221} & q_{222} \end{pmatrix}$ satisfies $Q\mathbf{x}^{(2)} = \mathbf{x}$ for every $\mathbf{x} \in \Omega_n$. If $R = [Q|Q]$, then $R\mathbf{x}^{(3)} = \mathbf{x}^{(3)} = \mathbf{x}$ for every $\mathbf{x} \in \Omega_n$. Now, observe that the entries of $\mathbf{x}^{(3)}$ indexed by 112, 121, 211 are all equal to $x_1^2x_2$. So, we can permute the columns of R indexed by 112, 121, 211 in $3! = 6$ different ways to get a matrix with the desired properties. Similarly, we can permute the columns of R indexed by 122, 212, 221 to get different matrices with the desired properties. As a result, we get $6^2 = 36$ different matrices with the desired property. Now, we can take convex combination these matrices to get a large family of matrices with the desired property.

One easily extends the above idea to obtain the following.

Theorem 3.1 *Suppose $m, n \geq 2$, and P is a transition probability tensor P represented as an $n \times n^m$ matrix such that $P\mathbf{x}^m = \mathbf{x}$ for all $\mathbf{x} \in \Omega_n$. Let $Q = [P|\dots|P] = \mathbf{1} \otimes P$ with $\mathbf{1} = (1, \dots, 1)$ with m copies. Then*

$$Q\mathbf{x}^{(m+1)} = (\mathbf{1} \otimes P)(\mathbf{x} \otimes \mathbf{x}^{(m)}) = (\mathbf{1}\mathbf{x}) \otimes (P\mathbf{x}^{(m)}) = \mathbf{x} \quad \text{for all } \mathbf{x} \in \Omega_n. \quad (5)$$

Moreover, one can permute the columns of Q corresponding to the entries in the vector $\mathbf{x}^{(m+1)}$ with the same values: $x_1^{m_1} \dots x_n^{m_n}$ for all nonnegative sequence (m_1, \dots, m_n) with $m_1 + \dots + m_n = m$ to yield other Markov chains satisfying (5); in addition, taking convex combination of these matrices will also result in Markov chains satisfying (5).

Note that there are

$$\binom{m}{m_1, m_2, \dots, m_n} = \frac{m!}{m_1! \dots m_n!}$$

so many terms in the vector $\mathbf{x}^{(m)}$, and hence there are $\binom{m}{m_1, m_2, \dots, m_n}!$ permutations for the corresponding columns in Q . Thus, we can generate many new matrices \tilde{Q} from Q satisfying $\tilde{Q}\mathbf{x}^{(m+1)} = \mathbf{x}$ for all $\mathbf{x} \in \Omega_n$.

An interesting question is whether a higher-order Markov chain with transition tensor Q satisfying $Q\mathbf{x}^{(m)} = \mathbf{x}$ for every $\mathbf{x} \in \Omega_n$ can be obtained from the above construction.

Next, we turn to higher-order Markov chains satisfying condition (II).

Theorem 3.2 Suppose $n > 2$ and an m -th order Markov chain with transition tensor $P = (p_{i_1, \dots, i_m})$ identified as and $n \times n^m$ matrix. Partition $P = [P_1 | \dots | P_n]$ so that the P_i is $n \times n^{m-1}$. Let $k \in \{1, \dots, n\}$ and $f_k = (e_1 + \dots + e_k)/k$. If every column of P_i equals f_k , then f_k is the only stationary vector of the Markov chain.

- (1) If $k = 2$, replace the first volume of P_1 by e_1 and replace all the columns of P_2 by e_2 . Then the resulting Markov chain has 2 stationary vectors, namely, e_1 and e_2 .
- (2) If $2 < k \leq n$, replace the column of P_i indexed by $(i_1, \dots, i_m) = (i, \dots, i)$ by e_i for all $i = 1, \dots, k$, and all other columns by e_k for $i = 1, \dots, k$, then the resulting Markov chain has k stationary vectors, namely, e_1, \dots, e_k .
- (3) Suppose $k = n$. If we replace the the column of P_i indexed by $(i_1, \dots, i_m) = (i, \dots, i)$ for all $i = 1, \dots, n$, then the resulting Markov chain has $n + 1$ stationary vectors, namely, e_1, \dots, e_n and f_n .
- (4) If $k \in \{2, \dots, n - 1\}$ and we replace the columns of P_i indexed by (i_1, \dots, i_m) with $1 \leq i_1, \dots, i_m \leq k$ by e_i for $i = 1, \dots, k$, then the set of stationary vectors for the Markov chain equals the convex hull of $\{e_1, \dots, e_k\}$.
- (5) Suppose $k \in \{2, \dots, n - 1\}$ and we reset the matrices P_1, \dots, P_n so that for each $i = 1, \dots, n$, the columns of P_i indexed by (i_1, \dots, i_m) with $1 \leq i_1, \dots, i_m \leq k$, equal

$$v_i = \begin{cases} e_i & \text{if } i = 1, \dots, k, \\ (e_{k+1} + \dots + e_n)/(n - k) & \text{if } i = k+1, \dots, n, \end{cases}$$

and all other columns of P_i equal f_n . Then the set of stationary vectors for the Markov chain equals the union of the convex hull of $\{e_1, \dots, e_k\}$ the set $\{f_n\}$.

Proof. The proof is an easy adaptation of that of Theorem 2.3. □

To conclude our note, we remark that there are many interesting questions concerning the stationary vectors of higher-order Markov chains that deserve further study.

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